4-Hydroxyphenylacetate

3233-32-7 | DTXSID70186062

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 93.5 °C

Global applicability domain: Inside

Local applicability domain index: 8.55e-01

Confidence level: 5.61e-01

Nearest Neighbors from the Training Set

Image not found
Methylparaben
Measured: 131
Predicted: 98.7

Image not found
Methyl 3-hydroxybenzoate
Measured: 73.0
Predicted: 95.8

Image not found
Ethylparaben
Measured: 117
Predicted: 101

Image not found
Ethyl 3-hydroxybenzoate
Measured: 74.0
Predicted: 93.5